

Computing eigenvalues of normal matrices via complex symmetric matrices

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Abstract

Computing all eigenvalues of a modest size matrix typically proceeds in two phases. In a first phase, the matrix is transformed to a suitable condensed matrix format, sharing the eigenvalues, and in the second stage the eigenvalues of this condensed matrix are computed. The main purpose of this intermediate matrix is saving valuable computing time. Important subclasses of normal matrices, such as the Hermitian, skew-Hermitian and unitary matrices admit a condensed matrix represented by only $O(n)$ parameters, allowing subsequent low-cost algorithms to compute their eigenvalues. Unfortunately, such a condensed format does not exist for a generic normal matrix.

We will show, under modest constraints, that normal matrices also admit a memory cheap intermediate matrix of tridiagonal complex symmetric form. Moreover, we will propose a general approach for computing the eigenvalues of a normal matrix, exploiting thereby the normal complex symmetric structure. An analysis of the computational cost and numerical experiments with respect to the accuracy of the approach are enclosed. In the second part of the manuscript we will investigate the case of nonsimple singular values and propose a theoretical framework for retrieving the eigenvalues. We will, however, also highlight some numerical difficulties inherent to this approach.

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Computing eigenvalues of normal matrices via complex symmetric matrices [☆]

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Abstract

Computing all eigenvalues of a modest size matrix typically proceeds in two phases. In the first phase, the matrix is transformed to a suitable condensed matrix format, sharing the eigenvalues, and in the second stage the eigenvalues of this condensed matrix are computed. The main purpose of this intermediate matrix is saving valuable computing time. Important subclasses of normal matrices, such as the Hermitian, skew-Hermitian and unitary matrices admit a condensed matrix represented by only $O(n)$ parameters, allowing subsequent low-cost algorithms to compute their eigenvalues. Unfortunately, such a condensed format does not exist for a generic normal matrix.

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Keywords: normal matrix, complex symmetric, Takagi factorization, unitary similarity, symmetric singular value decomposition, eigenvalue decomposition

1. Introduction

Most of the so-called direct eigenvalue methods are based on a two-step approach. First the original matrix is transformed to a suitable shape taking $O(n^3)$ operations, followed by the core method computing the eigenvalues of this suitable shape, e.g., divide-and-conquer, MRRR, QR -methods [10, 22, 23]. Consider, e.g., the QR -method; starting with an arbitrary unstructured matrix, one first performs a unitary similarity transformation to obtain a Hessenberg matrix in $O(n^3)$ operations. Next, successive QR -steps, which cost $O(n^2)$ each, are performed until all eigenvalues are revealed.

For some subclasses of normal matrices, e.g., Hermitian, skew-Hermitian, and unitary matrices, the intermediate matrix shapes admit a low storage cost $O(n)$ and, as such, permit the design of QR -algorithms with linear complexity steps [1, 3, 22]. Unfortunately, for the generic normal matrix class, the intermediate structure is of Hessenberg form, requiring $O(n^2)$ storage and resulting in a quadratic cost for each QR -step. An alternative intermediate condensed form might thus result in significant computational savings. To achieve this goal we propose the use of intermediate complex symmetric matrices that can be constructed using unitary similarities. The problem of determining whether a

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square complex matrix is unitarily similar to a complex symmetric one has been intensively studied; see, for instance, [2, 8, 21]. Such a similarity always exists for normal matrices [12, Corollary 4.4.4]. One method to perform the unitary transformation of a normal matrix to complex symmetric form was proposed by Ikramov in [13]. It utilizes the Toeplitz decomposition of the normal matrix and symmetries at the same time the two Hermitian terms.

The aim of this article is to provide an initial theoretical basis on which we can continue to build numerical algorithms. Again we rely on the two-step principle: First, the matrix is transformed by a unitary similarity transformation to block matrix form, of which the diagonal blocks are complex symmetric. In the simplest case only one block exists [20], and well-known techniques [4, 24, 25] can be used to compute the symmetric singular value decomposition (SSVD), also called Autonne-Takagi factorization [12, 18], of this complex symmetric matrix. Based on the SSVD one can retrieve the eigenvalue decomposition. When multiple blocks are present, it is possible to use the same techniques and diagonalize all blocks at once, obtaining a sparse matrix with all blocks diagonal. After that, a specifically designed version of the Jacobi method for normal matrices [9, 17, 19] is used, in order to annihilate the last nonzero off-diagonal entries. Numerical experiments illustrate the effectiveness of the proposed method. Whenever the number of block exceeds one, it will be shown, however, that severe numerical difficulties can appear. More precisely, many articles and authors rely on the property that an irreducible Hermitian tridiagonal matrix cannot have coinciding eigenvalues. Though theoretically correct, this statement might fail in a numerical setting, with nonnegligible impact on the accuracy of the proposed methods (see Section 6 or the discussion in [23, Section 5.45]).

In this article, the following notation is used: A^T refers to the transpose of A , \bar{A} to the conjugate of A and $A^H = \bar{A}^T$ denotes the Hermitian conjugate. With $A(i : j, \ell : k)$ the submatrix of a matrix A consisting of rows i up to and including j and columns ℓ up to and including k is depicted. With a_i we refer to the i -th column of A . A matrix is said to be symmetric if $A = A^T$ and Hermitian if $A = A^H$. A matrix is real orthogonal if $AA^T = A^T A = I$ and A is real, and unitary if $AA^H = A^H A = I$. We might use the expressions real and complex symmetric to stress that the symmetric matrix is real or possibly complex. The elements of a matrix A are denoted by a_{ij} , when taking subblocks out of a partitioned matrix, we refer to them as A_{kl} . The square root of -1 is denoted by ι .

The article is organized in two main parts. One part of the article discusses the easy setting in which the intermediate matrix is of complex symmetric form. The second part of the article presents a theoretical approach to deal with the block form, and discusses possible numerical issues. Section 2 recapitulates some known results on normal matrices, the singular value decomposition and results from [20]. In Section 3, under some constraints, the theoretical setting for eigenvalue computations of normal matrices whose distinct eigenvalues have distinct absolute values is considered. The unitary similarity transformation as well as the link with the SSVD is presented to reveal the eigenvalues. Section 4 supports the theoretical discussion by numerical experiments. In Section 5 the generic nonsingular case is investigated. The similarity transformation will now result in a block structured matrix, which can be diagonalized efficiently. The eigenvalues of this latter sparse block matrix are then computed via a Jacobi-like diagonalization procedure. In Section 6 some numerical experiments and observations with respect to the latter structure are presented. We also compare the performance of our method with that of [13] in relation to different distributions of eigenvalues and singular values: we show that both methods can suffer from discrepancies between their theoretical and practical behavior.

2. Preliminaries

This section highlights some essential properties of normal matrices, the singular value decomposition, and some other results required in the remainder of the text.

A singular value decomposition of A is a factorization of the form $A = U\Sigma V^H$, where U, V are unitary matrices, and Σ is a diagonal matrix with nonnegative real entries $\sigma_1, \dots, \sigma_n$, we write $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$. The diagonal elements of Σ are called the singular values of A and the columns of U and V are called the left and right singular vectors respectively. A singular value σ_i is said to be a multiple singular value if it appears more than once on the diagonal of Σ . A standard choice consists of ordering the singular values such that $\sigma_1 \geq \dots \geq \sigma_n$ [10]. We will implicitly assume that every singular value decomposition in this article has this conventional form, except when stated otherwise, and we will stress this by naming it an unordered singular value decomposition. It is well-known that the singular value decomposition for a matrix with n distinct singular values is essentially unique [10], which signifies unique up to unimodular scaling. The unordered version is also unique up to permutations of the diagonal element as long as the singular values are unique.

Suppose that the matrix has singular values of multiplicities exceeding one, so that uniqueness is lost. One then still has uniqueness of the subspaces associated with equal singular values, as given by the following theorem.

Lemma 1 (Autonne's uniqueness theorem, Theorem 2.6.5 in [12]). *Let $A \in \mathbb{C}^{n \times n}$ and let $A = U\Sigma V^H = W\Sigma Z^H$ be two, possibly distinct, singular value decompositions. Then there exist unitary block diagonal matrices $B = \text{diag}(B_1, B_2, \dots, B_d)$ and $\tilde{B} = \text{diag}(\tilde{B}_1, \tilde{B}_2, \dots, \tilde{B}_d)$, such that $U = WB$, $V = Z\tilde{B}$ and $B_i = \tilde{B}_i$ whenever the associated singular value differs from zero.*

In general, given a matrix $A \in \mathbb{C}^{n \times n}$ and a singular value decomposition $A = U\Sigma V^H$, we have that $AA^H = U\Sigma^2 U^H$ and $A^H A = V\Sigma^2 V^H$ are eigenvalue decompositions of AA^H and $A^H A$ respectively, having orthonormal eigenvectors. If $A \in \mathbb{C}^{n \times n}$ is normal, then $AA^H = A^H A$, so the columns of U and V both form a basis of \mathbb{C}^n , made out of eigenvectors of the same matrix. This means that all columns of U and all columns of V stemming from an identical, possibly multiple, singular value must span the same eigenspace of AA^H .

The existence of an eigenvalue decomposition with orthogonal eigenvectors, is equivalent to being normal.¹ So for a normal matrix A having an eigenvalue decomposition $A = Q\Lambda Q^H$, where $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$ and $QQ^H = I$, we can always obtain a singular value decomposition. Simply consider matrices $\Sigma = \text{diag}(|\lambda_1|, \dots, |\lambda_n|)$ and $\bar{\Omega} = \text{diag}(e^{i\theta_1}, \dots, e^{i\theta_n})$, where $\lambda_i = |\lambda_i|e^{i\theta_i}$, for all $i = 1, \dots, n$. Then $A = Q\Sigma(Q\bar{\Omega})^H$ is an unordered singular value decomposition.

Remark 2. Consider a polar decomposition $A = PW$ of $A \in \mathbb{C}^{n \times n}$, i.e., a factorization where P is Hermitian positive semidefinite and W is unitary. Let $P = U\Sigma U^H$ be a unitary² eigenvalue decomposition of P . Then $A = U\Sigma(W^H U)^H$ is an unordered singular value decomposition of A . A matrix is normal if and only if its polar factors commute [11]. Hence, If A is normal, its polar decomposition provides us two possibly different unordered singular value decompositions: $A = U\Sigma(W^H U)^H = (WU)\Sigma U^H$.

In [20] the following theorem was proved, serving as a basis for the investigations proposed in this article.

Theorem 3 (Theorem 1 in [20]). *Let $A \in \mathbb{C}^{n \times n}$ be a normal matrix, having distinct singular values and $A = UB V^H$, with U, V unitary and B a real matrix. Then $A_U = U^H A U$ and $A_V = V^H A V$ will be symmetric matrices.*

The algorithm proposed in [20] relies on the standard bidiagonalization procedure to compute U , V , and B , and it allows the use of a real orthogonal transformation when A is real. However, as we are going to show in Subsection 3.1, the same result is possible with less strict demands; in particular it is shown that bidiagonal matrix B is not required.

3. Eigenvalue retrieval of normal matrices unitarily similar to a symmetric one

This section proposes an alternative approach, not relying on an intermediate Hessenberg matrix, for computing the eigenvalues of a normal matrix whose distinct eigenvalues have distinct absolute values. The more general setting is presented in Section 5.

3.1. Unitary similarity transform to symmetric form

A construction of a unitary similarity transformation to complex symmetric form was discussed in [20]. In that article the normal matrix was assumed to have distinct singular values. The proof of Theorem 3 was explicitly based on the construction of the complex symmetric matrix and used the intermediate matrix B . However, the matrix B is theoretically redundant, and one can formulate more general versions of Theorem 3.

Lemma 4. *Let $A \in \mathbb{C}^{n \times n}$ be a normal matrix. Then AA^H is real if and only if*

$$A = Q \text{diag}(\sigma_1 W_1, \dots, \sigma_d W_d, 0_{n-r}) Q^T,$$

where $\sigma_1, \dots, \sigma_d$ are the distinct positive singular values of A , $r = \text{rank}(A)$, W_i is unitary for each $i = 1, \dots, d$, and Q is a real orthogonal matrix.

¹There is an extended list of properties equivalent to being normal, see, e.g., [6, 11].

²A unitary (real orthogonal) eigenvalue decomposition is an eigenvalue decomposition whose matrix of eigenvectors is unitary (real orthogonal).

Proof. If $A = Q \text{diag}(\sigma_1 W_1, \dots, \sigma_d W_d, 0_{n-r}) Q^T$, then AA^H is trivially real. Let us consider the other implication. Let $A = PW$ be a polar decomposition of A . Then $P^2 = AA^H$ is real, so also P must be real. Consider a real orthogonal eigenvalue decomposition $P = Q\Sigma Q^T$. Then

$$\Sigma = \text{diag}(\sigma_1 I_{n_1}, \dots, \sigma_d I_{n_d}, 0_{n-r}),$$

where $r = \text{rank}(A)$, and n_i is the multiplicity of σ_i . An unordered singular value decomposition of A is given by $A = Q\Sigma(Q^T W)$, and by Remark 2 also $A = (WQ)\Sigma Q^T$ is one. By Lemma 1, we find

$$Q^T W Q = \text{diag}(W_1, \dots, W_d, W_{d+1}).$$

Replacing W by $Q \text{diag}(W_1, \dots, W_d, W_{d+1}) Q^T$ in the polar decomposition, we have that

$$A = Q\Sigma \text{diag}(W_1, \dots, W_d, W_{d+1}) Q^T = Q \text{diag}(\sigma_1 W_1, \dots, \sigma_d W_d, 0_{n-r}) Q^T.$$

□

The previous result provides fundamental information showing that, once we require AA^H to be real, a normal matrix A is symmetric if and only if every W_i from Lemma 4 is unitary and symmetric. We are now interested in determining conditions under which this property holds. A first sufficient condition is straightforward.

Corollary 5. *Let $A \in \mathbb{C}^{n \times n}$ be a normal matrix having its positive singular values distinct (multiplicities one), and suppose AA^H is real. Then A is symmetric.*

Proof. Write A in the form $A = Q \text{diag}(\sigma_1 W_1, \dots, \sigma_d W_d, 0_{n-r}) Q^T$. The positive singular values have multiplicity one, so the unitary matrices W_i are of size 1×1 for each $i = 1, \dots, d$, implying symmetry. □

The previous corollary clearly extends Theorem 3. Indeed, if B is real, then $A_U A_U^H = BB^H$ is also real, and A_U is symmetric. The same holds for A_V . Furthermore Lemma 4, and thus also Corollary 5, are still valid when 0 is a multiple singular value, no matter how large its multiplicity. Corollary 5 can be generalized even further.

Corollary 6. *Let $A \in \mathbb{C}^{n \times n}$ be normal and suppose that distinct eigenvalues of A (possible higher multiplicity) have distinct absolute values. If AA^H is real, then A is symmetric.*

Proof. Write A in the form $A = Q \text{diag}(\sigma_1 W_1, \dots, \sigma_d W_d, 0_{n-r}) Q^T$. Each unitary matrix W_j has only one eigenvalue $e^{i\theta_j}$ with multiplicity n_j , so $W_j = e^{i\theta_j} I_{n_j}$ for each $j = 1, \dots, d$, implying symmetry. □

We can now generalize the results of Theorem 3.

Theorem 7. *Let $A \in \mathbb{C}^{n \times n}$ be a normal matrix and $A = UBV^H$, with U, V unitary and B a real matrix. If distinct eigenvalues of A have distinct absolute values, then $A_U = U^H A U$ and $A_V = V^H A V$ are symmetric normal matrices.*

Proof. Both $A_U A_U^H = BB^H$ and $A_V A_V^H = B^H B$ are real matrices and their eigenvalues are equal to those of A . Thus Corollary 6 holds for A_U and A_V , implying symmetry. □

Example 8. To clarify the meaning of the previous results, we include a practical example. Consider the normal matrix

$$A = \begin{bmatrix} iI_2 & -I_2 \\ I_2 & iI_2 \end{bmatrix}.$$

The eigenvalues of A are 0 and $2i$, both with multiplicity 2. Use the reduction proposed in [20] to get the unitary matrix V such that $A_V A_V^H$ is real, where $A_V = V^H A V$. The matrix A_V has the same eigenvalues as A , and they comply with the hypothesis of Corollary 6. We obtain

$$V = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & -i & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \text{ and } A_V = \begin{bmatrix} i & i & 0 & 0 \\ i & i & 0 & 0 \\ 0 & 0 & i & i \\ 0 & 0 & i & i \end{bmatrix},$$

the last one being clearly symmetric.

This result strongly depends on the eigenvalues as required in the hypothesis. It does not need to hold when distinct eigenvalues share the same modulus: see, e.g., Example 13.

However, if AA^H is real, it is always possible to determine if A is symmetric, even when the distribution of the eigenvalues is unknown. The following theorem shows a necessary and sufficient condition for the symmetry of A .

Theorem 9. *Let $A \in \mathbb{C}^{n \times n}$ be normal and suppose that AA^H is real. Then A is symmetric if and only if $AA^H = A\bar{A}$.*

Proof. Consider A in the form $A = Q \text{diag}(\sigma_1 W_1, \dots, \sigma_d W_d, 0_{n-r}) Q^T$ from Lemma 4. The matrices W_i are unitary; they are thus symmetric if and only if $W_i \bar{W}_i = I_{n_i}$ for each $i = 1, \dots, d$. That is equivalent to

$$AA^H = Q \text{diag}(\sigma_1^2 I_{n_1}, \dots, \sigma_d^2 I_{n_d}, 0_{n-r}) Q^T = A\bar{A}.$$

□

We can reconsider now the sufficient conditions on the eigenvalues required in Corollaries 5, 6, and Theorem 7. As we saw, they ensured the matrices W_i to be unitary diagonal, trivially implying that $AA^H = A\bar{A}$. They are thus particular cases in which the condition of Theorem 9 is satisfied.

Even though the constraint $AA^H = A\bar{A}$ allows us to treat most of normal matrices, some particular important subclasses do not possess this property. For instance, it does not hold for generic real orthogonal and unitary non-symmetric matrices, or for nonzero real skew-symmetric matrices. The development of a new numerical method for computing eigenvalues implies hence also the capability of dealing with these matrices, which is proposed in Section 5.

3.2. Exploiting the symmetric singular value decomposition to retrieve the eigenvalues

Even if the condition $AA^H = A\bar{A}$ is sufficient to ensure the symmetry, it does not ensure essentially uniqueness of the singular value decomposition. In this section we rely on additional constraints in order to exploit the symmetric structure to compute an eigenvalue decomposition of A . We suppose for now that the normal matrix A under consideration complies with the assumptions in Theorem 7 (distinct eigenvalues have distinct absolute values), the other case is discussed in Section 5. Both the normality and the symmetric structure play an essential role in constructing the new algorithm. Let us consider some decompositions for both normal and symmetric matrices and design an algorithm based on them.

Normal matrices. Suppose that A is normal, admitting a singular value decomposition $A = U\Sigma V^H$, and an eigenvalue decomposition $A = Q\Lambda Q^H$. As we showed, with a suitable permutation Π , $\Lambda\Pi = \Sigma\Omega$, with Ω a unitary diagonal matrix containing the arguments of all eigenvalues and Σ containing the moduli. In fact we have $A = Q\Lambda Q^H = U\Sigma\Omega(V\Omega)^H$. This implies, once we know the singular value decomposition, that under the conditions imposed on the normal matrices, $\Omega = V^H U$ (see proofs of Corollary 5 and Corollary 6), which can be used to retrieve the eigenvalues. Unfortunately computing both a left and right set of singular vectors is quite expensive.

Symmetric matrices. A complex symmetric matrix A is not normal in general, but always admits a so-called symmetric singular value decomposition (SSVD), often also named a Takagi or Autonne-Takagi factorization [12, 18]. This factorization has the form: $A = W\Sigma W^T$, where Σ is a diagonal matrix containing the singular values and W is a unitary matrix: $WW^H = W^H W = I$. It is clear that this is a special type of singular value decomposition. What makes an SSVD particularly interesting is the fact that complex conjugates of singular vectors are left singular vectors. Thus, only one set of singular vectors should be computed leading to an overall reduction of the computational cost, generally depending on the method used to compute the SSVD (see Section 4.1), and of the storage costs.

Normal and symmetric. If the matrix A is both normal and complex symmetric, we have the possibility to combine the two decompositions. Once we have computed an SSVD $A = W\Sigma W^T$, we can always obtain the eigenvalue decomposition $A = W(\Sigma\Omega)W^H$, as for the generic normal matrix, but this time computing the moduli of the eigenvalues is much more attractive. Computing the diagonal matrix $\Omega = W^T W$ requires only one set of right (or left) singular vectors.

The entire algorithm for a normal matrix whose distinct eigenvalues have distinct moduli can therefore be summarized in three steps:

- Apply a first transformation to obtain a symmetric matrix A , see [20];
- use one of the well-known methods to compute an SSVD factorization $A = W\Sigma W^T$. There exist several ways to manage this problem, see e.g., [4, 24, 25] and Section 4 where they are briefly discussed;
- compute the diagonal matrices $\Omega = W^T W$ and $\Lambda = \Sigma\Omega$. The factorization $A = W\Lambda W^H$ is then an eigenvalue decomposition of A .

4. Numerical experiments

In this section, we first compare the theoretical cost of the proposed method with that of the generic QR algorithm. Thereafter, we present the results of some numerical experiments in order to investigate the accuracy of the algorithm. We implemented our algorithm relying on both the twisted factorization method [25] and the QR-based method [5] to compute the SSVD of a symmetric matrix.³ We observed in some preliminary tests that these two approaches outperform the divide-and-conquer approach [24] in terms of accuracy.

4.1. Complexity analysis

Both the methods proposed in [5, 25] for computing the SSVD must be applied to symmetric tridiagonal matrices. Hence an additional transformation to symmetric tridiagonal form is required, e.g., by Householder transformations. The overall algorithm for the eigenvalue retrieval consists of four steps:

- **CS**: transformation of a normal matrix A to normal symmetric form C : $A = U_1 C U_1^H$;
- **TRI**: transformation of the normal symmetric matrix to (possibly not normal) symmetric tridiagonal form: $C = U_2 T U_2^T$;
- **TF**: computation of the SSVD: $T = U_3 \Sigma U_3^T$;
- **ED**: retrieval of the eigenvalue decomposition based on the SSVD: $A = U \Lambda U^H$.

Let us consider in detail the costs of the individual steps and compare the resulting complexity with that of the classical QR method. In the following we will always omit lower order terms and consider only the dominant terms. The first step requires $\frac{8}{3}n^3$ flops for the bidiagonalization, $8n^3$ flops for computing C . The second step requires $\frac{4}{3}n^3$ flops for the tridiagonalization and $2n^3$ additional flops for computing U_2 . The transformation of a normal matrix to complex symmetric tridiagonal form thus has a total cost of $12n^3$ flops.

The cost of the third step strongly depends on the selected method. The QR-based approach translates the algorithm for computing the singular values of a bidiagonal matrix to the tridiagonal setting. As one relies on the QR factorization of TT^H , this results in a double shifted QR-step. This method needs $O(n^2)$ flops for computing singular values and $O(n^3)$ flops for computing the singular vectors if all operations are accumulated. On average, the total cost is $6n^3$ for computing the whole SSVD [16]. Alternatively, the twisted factorization method focuses on computing the singular vectors, assuming thereby that the singular values are known. This method is based on the MRRR algorithm for computing the eigenvectors of symmetric tridiagonal matrices [5]. It has a total complexity of $O(n^2)$ for computing the whole SSVD [25]. But it must be stressed that this holds only when all singular values are well separated. In practice, this method's accuracy suffers greatly from singular values being too close.

The fourth and last step has also a neglectable cost of $O(n^2)$, and $4n^3$ additional flops are necessary to apply U_2 to U_3 and U_1 to the obtained product. In conclusion, to compute the entire eigenvalue decomposition, we need $16n^3$ and $22n^3$ flops, utilizing the twisted factorization or QR-based method respectively. On the other hand, the classic QR method for generic matrices requires in total $25n^3$ for the average case [10].

³The code for computing the SSVD via these three different methods [5, 24, 25] was downloaded from Sanzheng Qiao's personal webpage.

4.2. Accuracy

In this section we present the results of some practical experiments. We build some normal matrices with evenly distributed singular values (minimal gap equal to 0.05), as we want to compare the performances of the QR based and the twisted factorization methods. Normal matrices with predetermined eigenvalues were generated as follows: given the vector λ containing the eigenvalues, the matrix A is defined as $A = Z \text{diag}(\lambda) Z^H$, where Z is a random unitary matrix obtained by the QR decomposition of a random complex matrix. For every size $n = 50, 100, \dots, 1500$ the same experiment is repeated three times, and the mean value is taken for every measured magnitude.

The errors in Figure 1 related to the individual steps were measured as

$$\Delta_{CS} = \frac{\|A - U_1 C U_1^H\|}{\|A\|}, \quad \Delta_{TRI} = \frac{\|C - U_2 T U_2^T\|}{\|C\|}, \quad \Delta_{SSVD}^{QR} = \frac{\|T - U_{QR} \Sigma U_{QR}^T\|}{\|T\|}, \quad \Delta_{SSVD}^{TF} = \frac{\|T - U_{TF} \Sigma U_{TF}^T\|}{\|T\|},$$

where $\|\cdot\|$ is the two-norm and "QR" and "TF" indicate if the singular vectors are obtained via the QR-based or the twisted factorization method respectively.

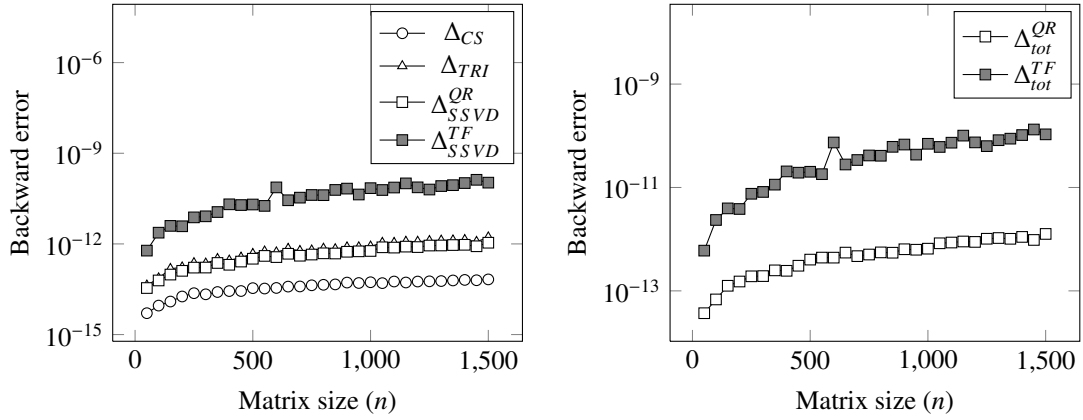


Figure 1: Backward errors of the single steps and of the total decomposition

The total backward error was measured as

$$\Delta_{tot} = \frac{\|A - U_1 U_2 U_3 \Sigma U_3^T U_2^T U_1^H\|}{\|A\|},$$

with U_3 varying, depending again on the method selected to perform the third step. These error measures reflect the accuracy of the entire decomposition, capturing both eigenvalues and eigenvectors.

The overall relative eigenvalue errors are then determined as

$$\Delta_\lambda = \max_{i=1,\dots,n} \left(\frac{|\lambda_i - \tilde{\lambda}_i|}{|\lambda_i|} \right), \quad \text{and} \quad \Delta_{\text{eig}} = \max_{i=1,\dots,n} \left(\frac{|\lambda_i - \hat{\lambda}_i|}{|\lambda_i|} \right),$$

where $\tilde{\lambda}_i$ are the computed eigenvalues, and $\hat{\lambda}_i$ are the eigenvalues computed by Matlab's `eig` command. In Figure 2, we compare different values of Δ_λ , depending on the method chosen for computing the SSVD, with the corresponding error Δ_{eig} .

5. The generic nonsingular normal case: intermediate block matrices

In the previous section, some constraints were put on the eigenvalues and singular values, to compute the eigenvalues of a normal matrix in an alternative manner. It is possible, however, to use similar techniques to compute the eigenvalue decomposition of an arbitrary nonsingular normal matrix. In this section, we will provide a framework, where the original matrix is first transformed to a suitable block form; next, all blocks are diagonalized simultaneously; and, finally, a global eigenvalue decomposition of the matrix is deduced.

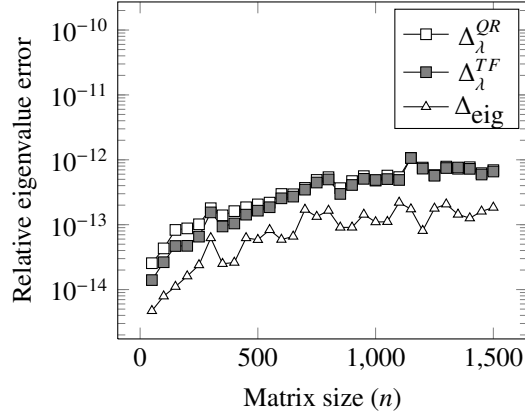


Figure 2: Relative eigenvalue errors

5.1. Unitary similarity transformation

Forthcoming Theorem 10 states that the algorithm for reducing a normal matrix to symmetric form always results in a block matrix, whose diagonal blocks are symmetric. The proof is based on a further specialization of the results from Theorem 3 and utilizes explicitly the reduction to bidiagonal form, because theoretically this can ensure the absence of multiple singular values. Suppose namely B to be a bidiagonal matrix, $B^H B$ then becomes an Hermitian tridiagonal matrix. It is well-known that an irreducible, i.e., having nonzero off-diagonal elements, Hermitian tridiagonal matrix must have distinct eigenvalues (see, for example, [10, Theorem 8.5.1] or [23, Section 5.37]). Hence, in the preprocessing step performing the unitary similarity transformation to complex symmetric form, one can easily detect nonsingularity and absence of singular values of a higher multiplicity as one passes via the bidiagonal form.

Furthermore, assume that the nonsingular normal matrix A has singular values σ_i , having multiplicities m_i . This implies that the resulting matrix B has at least $m = \max_i m_i - 1$ zeros on the superdiagonal. Moreover, in each of the diagonal blocks, all the singular values must be different from each other.

Theorem 10. *Let $A \in \mathbb{C}^{n \times n}$ be a nonsingular normal matrix and assume $A = UB^H$, with U, V unitary and B a real bidiagonal matrix. The indices $\{i_1, \dots, i_{m-1}\}$ indicate the rows i_ℓ for which the superdiagonal element $b_{i_\ell, i_\ell+1}$ equals zero (by definition we set $i_0 = 0$, and $i_m = n$).*

Then we have for $A_U = U^H A U$ and $A_V = V^H A V$ that the diagonal blocks $A_U(i_{\ell-1} + 1 : i_\ell, i_{\ell-1} + 1 : i_\ell)$ and $A_V(i_{\ell-1} + 1 : i_\ell, i_{\ell-1} + 1 : i_\ell)$ are symmetric for $\ell = 1, \dots, m - 1$.

The proof is based on a suitable partitioning of A_U . To ease the presentation of the proof we introduce a sort of block Hadamard product.

Definition 11. Assume a matrix partitioned in blocks $A = (A_{k\ell})_{k\ell}$ with $A_{k\ell} \in \mathbb{C}^{n_k \times n_\ell}$ and a set of square matrices $\Upsilon = \{\Upsilon_{k\ell}\}_{k\ell}$ with $\Upsilon_{k\ell} \in \mathbb{C}^{n_\ell \times n_\ell}$ are given. The block Hadamard product $C = A \circ_B \Upsilon$ is defined as the matrix C partitioned accordingly to A and having blocks $C_{k\ell} = A_{k\ell} \Upsilon_{k\ell}$.

We remark that $A_{k\ell}$ and $\Upsilon_{k\ell}$ need not have the same dimension since all blocks of $\Upsilon_{k\ell}$ are square. Moreover, in general it is not even possible to combine the blocks of $\Upsilon_{k\ell}$ in a matrix Υ .

Proof of Theorem 10. The proof is inspired by the one presented in [20, Theorem 1] and is subdivided in two parts here. First, different eigenvalue decompositions of $A_U A_U^H$ are derived, followed by an investigation of the connections between the eigenvectors. Assume $m > 1$, otherwise $i_1 = n$ so that Theorem 3 applies.

Eigenvalue decompositions of $A_U A_U^H$. Assume the factorization $B = U^H A V$ is given, with B bidiagonal, U and V unitary, and the indices i_ℓ satisfying the assumptions from the theorem. Partition A_U in blocks $(A_U)_{k\ell}$:

$$(A_U)_{k\ell} = A_U(i_{\ell-1} + 1 : i_\ell, i_{\ell-1} + 1 : i_\ell), \quad \forall k, \ell = 1, \dots, m - 1.$$

Furthermore let $n_k = i_k - i_{k-1} + 1$, this means that $(A_U)_{k\ell}$ is of dimension $n_k \times n_\ell$.

The following relations hold for the matrix product $A_U A_U^H$:

$$A_U A_U^H = (U^H A U) (U^H A^H U) = U^H A A^H U = (U^H A V) (V^H A^H U) = B B^H = T. \quad (1)$$

The matrix B is real nonsingular and bidiagonal implying that T is a real nonsingular symmetric tridiagonal matrix. The zero superdiagonal elements in the matrix B introduce zeros in the sub- and superdiagonal of T ($t_{i_\ell, i_\ell+1} = 0 = t_{i_\ell+1, i_\ell}$), making T reducible. The tridiagonal matrix is hence of block diagonal form with diagonal blocks $T_{\ell\ell} = T(i_{\ell-1} + 1 : i_\ell, i_{\ell-1} + 1 : i_\ell)$, where $\ell = 1, \dots, m-1$. Due to the ordering of the singular values in the matrix B , the diagonal blocks of T have all eigenvalues different from each other. The eigenvalue decomposition of each individual diagonal block $T_{\ell\ell}$ is therefore essentially unique. Consider an eigenvalue decomposition of $A_U = Q \Lambda Q^H$, where the eigenvalues in the diagonal matrix Λ are ordered accordingly to the matrix T . This means that the diagonal elements of $|\Lambda_{\ell\ell}|^2$ equal the eigenvalues of the tridiagonal block $T_{\ell\ell}$. The matrix $T_{\ell\ell}$ admits therefore an essentially unique eigenvalue decomposition of the form $T_{\ell\ell} = \hat{Q}_{\ell\ell} |\Lambda_{\ell\ell}|^2 \hat{Q}_{\ell\ell}^H$, with $\hat{Q}_{\ell\ell}$ real orthogonal. Combining the decompositions for each block $T_{\ell\ell}$, we get another eigenvalue decomposition of the matrix product $A_U A_U^H = \hat{Q} |\Lambda|^2 \hat{Q}^H$, where the blocks $\hat{Q}_{k\ell} = 0$ whenever $k \neq \ell$.

Since T is real $T = \bar{T}$, Equation (1) combined with the eigendecomposition of $A_U = Q \Lambda Q^H$ gives us three different eigendecompositions of the matrix product $A_U A_U^H$:

$$A_U A_U^H = \hat{Q} |\Lambda|^2 \hat{Q}^H, \quad (2)$$

$$A_U A_U^H = Q |\Lambda|^2 Q^H, \quad (3)$$

$$A_U A_U^H = T = \bar{T} = \bar{A}_U A_U^T = \bar{Q} |\Lambda|^2 \bar{Q}^T. \quad (4)$$

In the original proof of Theorem 3 (see [20], the case $i_1 = n$) all singular values of A were assumed distinct. Hence the diagonal of $|\Lambda|^2$ contained all distinct values and consequently all invariant eigenspaces are of dimension one implying essentially uniqueness of the eigenvectors. This resulted in the fact that $\bar{Q} = Q \Omega$ by combining (3) and (4), with Ω a unitary diagonal matrix, proving thereby that A_U is symmetric.

Here, in this setting we can have invariant subspaces of higher dimensions belonging to a single eigenvalue from $A_U A_U^H$. Since, however, the eigenvalues are ordered in blocks of distinct eigenvalues we know that the column vectors of the block $Q_{:, \ell} = Q(:, i_{\ell-1} + 1 : i_\ell)$ all belong to different invariant subspaces and are hence orthogonal.

Relations between the eigenvectors. To present a unified link between the matrices \hat{Q} , Q and \bar{Q} , some extra matrices are needed. Construct a binary matrix P with $p_{ij} = 1$ if $|\lambda_i|^2 = |\lambda_j|^2$, where $\Lambda = \text{diag}(\lambda_i)$, and partition it according to A_U . The fact that the blocks $|\Lambda_{\ell\ell}|^2$ have all eigenvalues distinct imposes extra structure on the matrix P . All diagonal blocks $P_{\ell\ell} \in \mathbb{R}^{n_\ell \times n_\ell}$ are square identity matrices, the matrices $P_{k\ell} \in \mathbb{R}^{n_k \times n_\ell}$ have at most one nonzero entry (equal to 1) in each row and column. One can see this as a combination of a permutation followed by real diagonal projection matrix containing ones or zeros on its diagonal. The matrix $P_{k\ell}$ provides, in fact, links between identical eigenvalues of the diagonal blocks of $A_U A_U^H$. Moreover, the matrix P is symmetric $P_{k\ell} = P_{\ell k}^T$.

Taking $P_{k\ell} P_{k\ell}^T = P_{k\ell} P_{\ell k}$ and $P_{\ell k} P_{\ell k}^T = P_{\ell k} P_{k\ell}$, we see that we get diagonal projection matrices (having either one or zero on the diagonal) of dimensions $n_k \times n_k$ and $n_\ell \times n_\ell$ respectively. An important relation is the following:

$$P_{kj} P_{j\ell} = P_{k\ell} (P_{\ell j} P_{\ell j}^T), \quad (5)$$

in words this means: P_{kj} links the eigenvalues of block $|\Lambda_{kk}|^2$ to the ones of $|\Lambda_{jj}|^2$, this is followed by a link to the eigenvalues of the block $|\Lambda_{\ell\ell}|^2$. Hence, we have a link between the block $|\Lambda_{kk}|^2$ and the block $|\Lambda_{\ell\ell}|^2$, which is given by $P_{k\ell}$. Unfortunately, during this transition some links might get lost and this is modeled by the projection operator $(P_{\ell j} P_{\ell j}^T)$ retaining only the relations in $P_{k\ell}$ which are also present in $P_{\ell j}$.

Based on (2) and (3) we know that the eigenvectors \hat{Q} and Q must be linked. To obtain the eigenvectors in Q from the ones in \hat{Q} , only restricted combinations of columns of \hat{Q} are allowed. Only the eigenvectors belonging to identical eigenvalues and hence to the same invariant subspace can be combined. Using the block Hadamard product and the matrix P , we can write this as $Q = \hat{Q} (P \circ_B \Omega)$, where Ω is a set of diagonal matrices $\Omega_{\ell k}$. This product indicates nothing else than taking linear combinations (due to the multiplication with the $\Omega_{\ell k}$) of eigenvectors linked to identical

eigenvalues (imposed by P) of the columns of \hat{Q} , such to obtain the eigenvectors of Q . The matrix $(P \circ_B \Omega)$ is unitary and partitioned according to A_U . We remark that the diagonal matrices $\Omega_{\ell k}$ can be singular. Using (2) and (3) we also get the following relation: $\bar{Q} = \hat{Q}(\overline{P \circ_B \Omega}) = \hat{Q}(P \circ_B \bar{\Omega})$. Combining (3) and (4) gives us $\bar{Q} = Q(P \circ_B \Upsilon)$, with Υ again a set of diagonal matrices. One can also verify that $(P \circ_B \Upsilon)$ is symmetric, since $I = Q^T \bar{Q} = Q^T Q(P \circ_B \Upsilon)$.

Since the matrix \hat{Q} is block diagonal we obtain the following equations:

$$Q_{\ell k} = \sum_{i=1}^m \hat{Q}_{\ell i} (P \circ_B \Omega)_{ik} = \hat{Q}_{\ell \ell} (P \circ_B \Omega)_{\ell k} = \hat{Q}_{\ell \ell} P_{\ell k} \Omega_{\ell k} \quad (6)$$

$$\bar{Q}_{\ell k} = \hat{Q}_{\ell \ell} P_{\ell k} \bar{\Omega}_{\ell k}. \quad (7)$$

This means in fact that the columns of $Q_{\ell k}$ and $\bar{Q}_{\ell k}$ are reordered and scaled columns of the matrix $\hat{Q}_{\ell \ell}$. Since there exists a diagonal matrix $\Gamma_{\ell k}$ such that $\Omega_{\ell k} = \bar{\Omega}_{\ell k} \Gamma_{\ell k}$ we get that $Q_{\ell k} = \bar{Q}_{\ell k} \Gamma_{\ell k}$ which is in fact $Q = \bar{Q} \circ_B \Gamma$. Equations (6) and (7) indicate that each block $Q_{\ell k}$ and $\bar{Q}_{\ell k}$ can be reconstructed by reshuffling and scaling the columns of $\hat{Q}_{\ell \ell}$. The converse statement is less powerful: some (perhaps none if $Q_{\ell k} = 0$) columns of $\hat{Q}_{\ell \ell}$ can be reconstructed by reshuffling and rescaling some columns of $Q_{\ell k}$. A similar statement holds between the columns of $Q_{\ell i}$ and $Q_{\ell j}$, we have for $Q_{\ell j} = \hat{Q}_{\ell \ell} P_{\ell j} \Omega_{\ell j}$ that $Q_{\ell j} P_{ji} = \hat{Q}_{\ell \ell} P_{\ell j} \Omega_{\ell j} P_{ji}$. Since $\Omega_{\ell j}$ is a diagonal matrix of dimension $n_j \times n_j$, there exists another diagonal matrix $\hat{\Omega}_{\ell i}$ of dimension $n_i \times n_i$ such that $\Omega_{\ell j} P_{ji} = P_{ji} \hat{\Omega}_{\ell i}$. Using (5) leads to:

$$Q_{\ell j} P_{ji} = \hat{Q}_{\ell \ell} P_{\ell j} P_{ji} \hat{\Omega}_{\ell i} = \hat{Q}_{\ell \ell} P_{\ell i} (P_{ij} P_{ij}^T) \hat{\Omega}_{\ell i} = Q_{\ell i} (P_{ij} P_{ij}^T) \hat{\Omega}_{\ell i}.$$

This means that some of the columns of $Q_{\ell j}$ are a scalar multiple of columns of $Q_{\ell i}$.

We now have everything to complete the proof. The $\ell \ell$ diagonal block of the matrix A_U is of the following form:

$$(A_U)_{\ell \ell} = Q_{\ell,:} \Lambda Q_{\ell,:}^H = Q_{\ell,:} \Lambda \bar{Q}_{\ell,:}^T = Q_{\ell,:} \Lambda (Q_{\ell,:} (P \circ_B \Upsilon))^T = Q_{\ell,:} \Lambda (P \circ_B \Upsilon) Q_{\ell,:}^T = \sum_{i=1}^m \sum_{j=1}^m Q_{\ell i} \Lambda_{ii} P_{ij} \Upsilon_{ij} Q_{\ell j}^T.$$

Instead of proving that the global sum is symmetric, we can even prove that each of the above terms will be symmetric. When $i = j$, we get: $Q_{\ell i} \Lambda_{ii} P_{ii} \Upsilon_{ii} Q_{\ell i}^T$, which is clearly symmetric (P_{ii} is diagonal). Consider now $i \neq j$, then we have a term of the form $Q_{\ell i} \Lambda_{ii} P_{ij} \Upsilon_{ij} Q_{\ell j}^T$. Again we use the existence of a $\hat{\Upsilon}_{ij}$ such that $P_{ij} \Upsilon_{ij} = \hat{\Upsilon}_{ij} P_{ij}$ to obtain the following:

$$\begin{aligned} Q_{\ell i} \Lambda_{ii} P_{ij} \Upsilon_{ij} Q_{\ell j}^T &= Q_{\ell i} \Lambda_{ii} \hat{\Upsilon}_{ij} P_{ij} Q_{\ell j}^T \\ &= Q_{\ell i} \Lambda_{ii} \hat{\Upsilon}_{ij} (Q_{\ell j} P_{ji})^T \\ &= Q_{\ell i} \Lambda_{ii} \hat{\Upsilon}_{ij} (Q_{\ell i} (P_{ij} P_{ij}^T) \hat{\Omega}_{\ell i})^T = Q_{\ell i} \Lambda_{ii} \hat{\Upsilon}_{ij} \hat{\Omega}_{\ell i} (P_{ij} P_{ij}^T) Q_{\ell i}^T. \end{aligned}$$

This term is clearly symmetric and hence also the complete sum $(A_U)_{\ell \ell}$ will be symmetric. \square

The proof presented here, relies strongly on the existence of a block diagonal eigenvalue decomposition of the matrix T , which one can assume to exist because we pass via the bidiagonalization procedure. It is therefore unknown yet, whether a general formalism as in Section 3.1 also holds in this case.

Question 12. Let $A \in \mathbb{C}^{n \times n}$ be nonsingular normal. Whenever AA^H is real, will A be a block matrix whose diagonal blocks are symmetric?

At least we know that the answer is affirmative in specific cases.

Example 13. Suppose that $A \in \mathbb{R}^{2n \times 2n}$ is a nonsingular skew-symmetric matrix. Consider the real orthogonal similarity transformation from Theorem 3, to obtain $C = U^T A U$. The skew-symmetry implies that all the eigenvalues are purely imaginary, appearing in conjugate pairs, and $AA^H = AA^T \neq A^2 = AA$. Thus in this case the condition in Theorem 9 does not hold. We know, however, that $C = (C_{ij})_{ij}$ is a 2×2 block matrix, for which the diagonal blocks are real symmetric.

The real orthogonal transformation preserves the skew-symmetry, hence $C_{ii}^T = C_{ii} = -C_{ii}$ for both $i = 1, 2$, implying C_{11} and C_{22} to be zero. On the other hand, $C_{21} = -C_{12}^T$. Therefore C is of the form

$$C = U^T A U = \begin{bmatrix} 0 & C_{12} \\ -C_{12}^T & 0 \end{bmatrix},$$

with only the diagonal blocks respecting the symmetric structure.

Example 14. Let $U \in \mathbb{C}^{n \times n}$ be a unitary nonsymmetric matrix. Thus $U U^H \neq U \bar{U}$ but $U U^H = I$ is real. All the singular values of U are equal to 1. The diagonal blocks under consideration have then size 1×1 , being thus trivially symmetric.

5.2. Simultaneous block diagonalization

If the matrix has multiple singular values related to distinct eigenvalues, we cannot directly apply the algorithm described in Section 3, because only the diagonal blocks have the symmetric structure we need. On the other hand, it is possible to apply another transformation to reduce this block matrix to a sparse and handier form.

Theorem 15. Let $A \in \mathbb{C}^{n \times n}$ be a nonsingular normal matrix. Let $A = U B V^H$ where B is real bidiagonal and U, V are unitary. Consider the matrix $C = U^H A U$ or $C = V^H A V$. Then, there exists a real orthogonal block diagonal matrix $Q = \text{diag}(Q_1, \dots, Q_m)$, such that $Q_i \in \mathbb{C}^{n_i \times n_i}$ for each $i = 1, \dots, m$ and $Q^T C Q$ has the same block structure as C , with every block of diagonal or permuted diagonal form.

Proof. Though the proof follows almost directly when considering a decent ordering of the diagonal blocks and singular values, combined with (6), we also provide a slightly different way of looking at the problem, closer to the proofs in Section 3.1.

Assume that $m > 1$, otherwise the statement holds trivially. Let $B = Q \Sigma Z^T$ be a singular value decomposition of B . Because of the structure of B , both Q and Z can be taken real orthogonal and block diagonal. If, for instance, $C = U^H A U$, then $C = Q \Sigma (Q^T W)$ is a singular value decomposition of C . Similar reasoning as in the proofs of Corollary 5 and Corollary 6 implies that $Q^T C Q$ is in the required form, with every block diagonal or permuted diagonal. \square

The previous result ensures that it is always possible to apply a transformation by a real orthogonal block diagonal matrix, to transform all the blocks of the original matrix to permuted diagonal form at once. If the diagonal blocks of B are maximal, meaning that each of them has the maximum possible number of distinct singular values of the original matrix, then we can guarantee diagonal blocks. In any case, the resulting matrix has a limited number of nonzero entries, placed in symmetric positions, yielding a significant reduction in the cost of the forthcoming diagonalization.

On the other hand, computing the matrix Q explicitly would be too expensive. One more attractive way to get the same result is exploiting the Takagi factorizations of the diagonal symmetric blocks of A (in case these factorizations are essentially unique), or by considering eigenvalue decompositions of the diagonal blocks of the matrix T in (4).

5.3. From block diagonal to diagonal form

It remains to bring the block matrix to diagonal form. In this section we focus on how to achieve this. We start by considering a block matrix with all the blocks in permuted diagonal form, and we show how to apply the classic Jacobi method for normal matrices, for a fast and accurate diagonalization.

In the literature there are many examples and variants of this classic method, whose oldest and simplest version was presented by Jacobi in 1846 [14]. The main idea for computing the eigenvalues of a symmetric matrix, consists of minimizing at every stage the sum of the squares of the off-diagonal elements. This is accomplished by a rotation, acting on a selected off-diagonal entry called pivot. The main differences between the various Jacobi methods are about the class of matrices they are able to deal with, and the strategy used to choose pivots. The most general instance is due to Goldstine and Horwitz [9], and allow us to work with every normal matrix. Given a generic normal matrix $A \in \mathbb{C}^{n \times n}$, one single step of the iteration can be summarized as follows:

- Choose a pivot a_{jk} that maximizes $|a_{jk}|^2 + |a_{kj}|^2$;

- compute

$$\omega = \frac{a_{jj} + a_{kk}}{2}, \quad \text{and} \quad \theta = \frac{1}{2} \arg \left(-\det \begin{bmatrix} a_{jj} - \omega & a_{jk} \\ a_{kj} & a_{kk} - \omega \end{bmatrix} \right);$$

- find ϕ and α such that

$$\gamma = e^{-i\theta} a_{jk} + e^{i\theta} \bar{a}_{kj}, \quad \phi = \frac{1}{2} \arctan \left(\frac{|\gamma|}{\operatorname{re} (e^{-i\theta} (a_{jj} - a_{kk}))} \right), \quad \text{and} \quad \alpha = \arg (\gamma);$$

- perform the unitary similarity transformation $A = G^H A G$, where the nontrivial part of G different from the identity is located in positions (j, k) , (j, j) , (k, j) , and (k, k) . Written as a 2×2 matrix, it equals

$$G_{jk} = \begin{bmatrix} \cos \phi & -e^{i\alpha} \sin \phi \\ e^{-i\alpha} \sin \phi & \cos \phi \end{bmatrix}$$

and acts on the j -th and k -th rows and columns of A .

Typically the Jacobi method is considered to be slow. In our setting, however, it serves as an adequate algorithm for zeroing the remaining off-diagonal elements. There are two big advantages. The rate of convergence of the Jacobi method is quadratic with respect to the number of entries that must be annihilated [15]. That is, in case of a dense matrix, proportional to $N = \frac{n(n-1)}{2}$, making the algorithm not suitable for large matrices. The situation is, however, different in our case, where the matrix has a limited number of nonzero off-diagonal entries: when all the blocks have, for instance, the same size $\frac{n}{k}$, the number of entries to annihilate is proportional to $N = \frac{n(k-1)}{2}$, resulting in a faster algorithm. This is not the only benefit: the entries that we want to eliminate follow a particular pattern, positioned on the permuted diagonals of a block matrix. As a result it is not necessary anymore to scan the entire matrix to select the pivot: when one nonzero element is found in a certain block, one does not need scan the rest of the row and column. Moreover, nonzero entries appear in symmetric position, so it is necessary to know only $\frac{n(n+1)}{2}$ entries to figure out their whole distribution. In addition, the transformations employed at every step do not create any fill-in because of the symmetry. We are thus able to reduce the cost of every step, performing the necessary multiplications only on the entries that are actually nonzero. All these expedients significantly reduce the overall cost.

An intriguing example is for instance a block matrix with only 4 blocks. This matrix can be diagonalized by a fixed number of rotators, namely the size of the off-diagonal block. The limited number of blocks causes the Jacobi method to sweep all nonzero elements away without adding new nonzero elements.

6. Numerical experiments

Though the theoretical setting to compute the eigenvalues of a nonsingular normal matrix relies mostly on reliable and quite efficient numerical techniques, there are some numerical issues. We would like to separate multiple eigenvalues, such that each diagonal block has no multiple eigenvalue left. Theoretically it is impossible to create an irreducible Hermitian tridiagonal matrix having multiple eigenvalues. This often brought the misleading idea that the eigenvalues can be considered reasonably distinct when none of the off-diagonal entries is particularly small.

On the contrary, it is numerically quite easy to get Hermitian tridiagonal matrices with pathologically close eigenvalues, in which none of the off-diagonal elements could be considered reasonably small. The Wilkinson matrix [23] is probably the most famous example of such matrices.

Example 16. Wilkinson matrices are real symmetric tridiagonal matrices having all the off-diagonal entries equal to 1, and diagonal entries $n, n-1, \dots, 1, 0, 1, \dots, n-1, n$, where $2n+1$ is the size of the matrix. So, for example, the Wilkinson matrix of size 5 is

$$W_5 = \begin{bmatrix} 2 & 1 & & & \\ & 1 & 1 & & \\ & & 1 & 0 & 1 \\ & & & 1 & 1 & 1 \\ & & & & 1 & 2 \end{bmatrix}.$$

What makes these matrices so peculiar is their distribution of eigenvalues: as the size grows larger, more and more pairs of eigenvalues get closer, while the off-diagonal entries remain constantly equal to 1. For instance, it is sufficient to choose $n = 10$ to get one pair of eigenvalues that agree up to 14 decimal places:

$$10.746194182903393 \text{ and } 10.746194182903322.$$

The previous example clearly illustrates that irreducibility of symmetric tridiagonal matrices does not imply, in practice, distinct eigenvalues, although it does in theory.

6.1. Symmetry

From a theoretical point of view, the new approach strongly relies on the bidiagonalization procedure, and on the presence of zero off-diagonal entries revealing multiple singular values. Also the symmetry of the diagonal blocks is closely related to the matrix B . The necessity to test this first step is thus essential.

In a first numerical experiment we want to test the sensitivity and robustness of the reduction procedure to symmetric form. The test matrices were generated as in Section 4, but this time we consider both matrices with random (uniformly distributed between 0 and 1) and equally spaced (minimal gap equal to 0.05) eigenvalues. The two plots in Figure 3 show the symmetry of C depending on the size of the problem, measured as

$$\Delta_s = \frac{\|C - C^T\|}{\|C\|}.$$

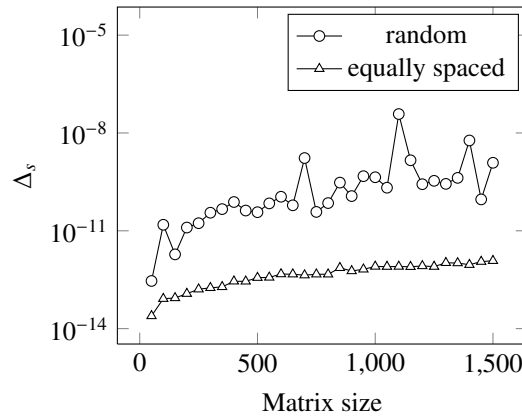


Figure 3: Symmetry of the matrix C for random and equally spaced eigenvalues.

Keeping in mind that “large” off-diagonal entries do not guarantee the eigenvalues to be distinct, we want to know how bad the consequences can be for the symmetrization methods. We considered both our and Ikramov’s method (DS) [13] to compute the unitary similarity to complex symmetric form. Both methods rely on the hypothetical zeros appearing on the off-diagonals to determine whether the matrix has multiple eigenvalues or not. Problems might arise when the eigenvalues of the considered matrices have some peculiar feature: for instance, the method presented in this paper could have difficulties in dealing with a normal matrix having distinct eigenvalues with equal absolute values; on the other hand, DS could fail if some eigenvalues have equal real or imaginary parts.

We present the results of two experiments concerning the two special settings mentioned above. The symmetry of the resulting matrix C was estimated as before. First we consider matrices having two pairs of eigenvalues with equal real and imaginary part respectively. These are not problematic for our method as long as their absolute values remain distinct. On the contrary, DS relies on the Toeplitz decomposition $N = H_1 + iH_2$ of the matrix; the current setting is thus troublesome, because both H_1 and H_2 have multiple eigenvalues. Indeed, the first plot in Figure 4 clearly shows that our method performs significantly better.

Next we consider matrices with one pair of distinct eigenvalues having the same absolute value. As we would expect DS performs well while our method occasionally works, as can be seen in the second plot. Note that this time the error is only related to the submatrix $C(1 : n - 1, 1 : n - 1)$ where n is the problem size, as we can only ensure a block structure.

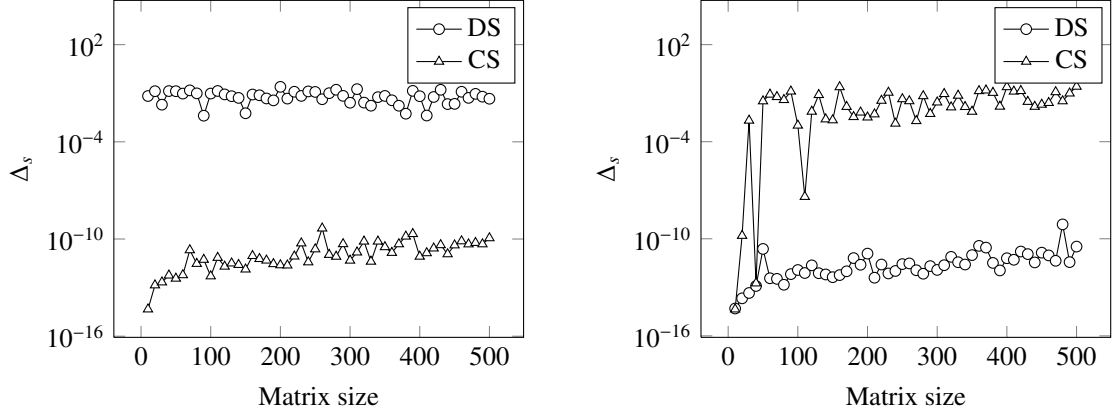


Figure 4: Comparing symmetry obtained in two special settings by our method and DS.

6.2. Accuracy

As we illustrated in the previous section, numerical issues can compromise the correct behavior of the method. Nonetheless the novel approach is quite satisfactory, with very good results in terms of accuracy for several problems. For instance, for normal matrices having one double singular value and minimum distance between distinct singular values equal to 1. We generated such kind of matrices as in Section 4, and computed eigenvalue decompositions of the diagonal blocks via the Takagi factorization as in Section 3.2 via twisted factorization or QR-based methods. The Jacobi method is then reduced to a single rotation, that annihilates the two nonzero off-diagonal entries.

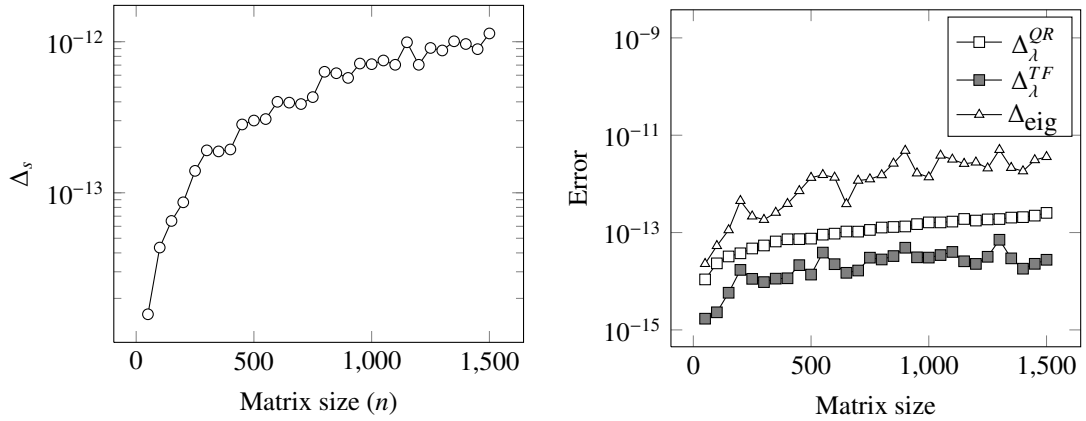


Figure 5: Symmetry of the matrix C and relative eigenvalue errors.

The new approach was proved to be reliable both in terms of symmetry of C and of accuracy of the computed eigenvalues, even outperforming Matlab's `eig` command results. Figure 5 shows an estimate of Δ_s , defined as in Section 6.1, and the trend of the eigenvalue error Δ_λ , defined as in Section 4, with respect to the size n of the matrix.

7. Conclusions and future work

In this article a novel approach to compute the eigenvalues of normal matrices was presented. The simplest case, where the intermediate matrix is symmetric, showed overall, good numerical performance, both with respect to speed as well as accuracy. The theoretical framework to process the more complex case seems promising, but can suffer significantly from numerical pitfalls.

The article opens several new directions for extending the current research. In Section 4 we relied entirely on existing algorithms to compute the SSVD factorization. These algorithms are constructed, however, for generic symmetric matrices and do not exploit the fact that the input matrix is also normal. We remark that normality is lost transforming the symmetric matrix to symmetric tridiagonal form.

Furthermore, a matrix is normal and symmetric if and only if it admits a real orthogonal eigenvalue decomposition, see [12, Problem 57, §2.5]. Unfortunately, the algorithm presented in this paper is not able to produce a real orthogonal matrix, except when the original matrix itself is real. Determining if it is possible to achieve the same result while using only real orthogonal transformations is still an open question.

The block case needs more attention: it is still unclear for which distribution of eigenvalues and singular values the method will work fine.

8. Acknowledgements

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9. Bibliography

- [1] G. S. Ammar, W. B. Gragg, and L. Reichel. On the eigenproblem for orthogonal matrices. In *Proceedings of the 25th IEEE Conference on Decision & Control*, pages 1963–1966. IEEE, New York, USA, 1986.
- [2] L. Balayan and S. R. Garcia. Unitary equivalence to a complex symmetric matrix. *Operators and Matrices*, 4:53–76, 2010.
- [3] A. Bunse-Gerstner and L. Elsner. Schur parameter pencils for the solution of the unitary eigenproblem. *Linear Algebra and its Applications*, 154-156:741–778, 1991.
- [4] A. Bunse-Gerstner and W. B. Gragg. Singular value decompositions of complex symmetric matrices. *Journal of Computational and Applied Mathematics*, 21:41–54, 1988.
- [5] I. S. Dhillon and B. N. Parlett. Multiple representations to compute orthogonal eigenvectors of symmetric tridiagonal matrices. *Linear Algebra and its Applications*, 387:1–28, 2004.
- [6] L. Elsner and Kh. D. Ikramov. Normal matrices: An update. *Linear Algebra and its Applications*, 285:291–303, 1998.
- [7] M. Fiedler. A characterization of tridiagonal matrices. *Linear Algebra and its Applications*, 2:191–197, 1969.
- [8] S. R. Garcia, D. E. Poore and M. K. Wyse. Unitary equivalence to a complex symmetric matrix: a modulus criterion. *Operators and Matrices*, 5:273–287, 2011.
- [9] H. H. Goldstine and L. P. Horwitz. A procedure for the diagonalization of normal matrices. *Journal of the ACM*, 6(2):195, 1959.
- [10] G.H. Golub and C. F. Van Loan. *Matrix Computations*. Johns Hopkins University Press, Baltimore, Maryland, USA, third edition, 1996.
- [11] R. Grone, C. R. Johnson, E. M. Sa, and H. Wolkowicz. Normal matrices. *Linear Algebra and its Applications*, 87:213–225, 1987.
- [12] R. A. Horn and C. R. Johnson. *Matrix Analysis*, 2nd ed.. Cambridge University Press, Cambridge, 2013.
- [13] Kh. Ikramov. Symmetrization of complex normal matrices. *Computational Mathematics and Mathematical Physics*, 33:837–842, 1993.
- [14] C. G. J. Jacobi. Über ein leichtes Verfahren, die in der Theorie der Säcularstörungen vorkommenden Gleichungen numerisch afzulösen. *Journal für die reine und angewandte Mathematik*, 30:51–94, 1846.
- [15] G. Loizou. On the quadratic convergence of the Jacobi method for normal matrices. *The Computer Journal*, 15(3):274, 1972.
- [16] F. T. Luk, S. Qiao. A fast singular value algorithm for Hankel matrices. *Fast Algorithms for Structured Matrices: Theory and Applications*, *Contemporary Mathematics*, 323:169–177, 2001.
- [17] A. Ruhe. Closest normal matrix finally found! *BIT*, 27:585–598, 1987.
- [18] T. Takagi. On an algebraic problem related to an analytic theorem of Carathéodory and Fejér and on an allied theorem of Landau. *Japanese Journal of Mathematics*, 1:82–93, 1924.
- [19] H. A. van der Vorst. *Computational methods for large eigenvalue problems*. Elsevier, North Holland, 2001.
- [20] R. Vandebril. A unitary similarity transform of a normal matrix to complex symmetric form. *Applied Mathematics Letters*, 24:160–164, 2011.
- [21] J. Vermeer. Orthogonal similarity of a real matrix and its transpose. *Linear Algebra and its Applications*, 428:382–392, 2008.
- [22] D. S. Watkins. *The Matrix Eigenvalue Problem: GR and Krylov Subspace Methods*. SIAM, Philadelphia, USA, 2007.

- [23] J. H. Wilkinson. *The Algebraic Eigenvalue Problem*. Oxford University Press, New York, USA, 1978.
- [24] W. Xu and S. Qiao. A divide-and-conquer method for the Takagi factorization. *SIAM Journal on Matrix Analysis and Applications*, 30(1):142–153, 2008.
- [25] W. Xu and S. Qiao. A twisted factorization method for symmetric SVD of a complex symmetric tridiagonal matrix. *Numerical Linear Algebra with Applications*, 16(10):801–815, 2009.